Bosons and fermions in external fields

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1 Introduction

In this article we discuss quantum theories which describe systems of non-distinguishable particles interacting with external fields. Such models are of interest also in the non-relativistic case (in quantum statistical mechanics, nuclear physics, etc.), but the relativistic case has additional, interesting complications: in the latter case they are genuine quantum field theories, i.e. quantum theories with an infinite number of degrees of freedom, with non-trivial features like divergences and anomalies. Since interparticle interactions are ignored, such models can be regarded as a first approximation to more complicated theories, and they can be studied by mathematically precise methods.

Models of relativistic particles in external electromagnetic fields have received considerable attention in the physics literature, and interesting phenomena like the Klein paradox or particle-antiparticle pair creation in over-critical fields have been studied; see [1] for an extensive review. We will not discuss these physics questions but only describe some proto-type examples

and a general Hamiltonian framework which has been used in mathematically precise work on such models. The general framework for this latter work is the mathematical theory of Hilbert space operators (see e.g. [2]), but in our discussion we try to avoid presupposing knowledge of that theory. As shortly mentioned in the end, this work has had close relations to various topics of recent interest in mathematical physics, including anomalies, infinite dimensional geometry and group theory, conformal field theory, and noncommutative geometry.

We restrict our discussion to spin-0 bosons and spin-$\frac{1}{2}$ fermions, and we will not discuss models of particles in external gravitational fields but only refer the interested reader to [3]. We also only mention in passing that external field problems have been also studied using functional integral approaches, and mathematically precise work on this can be found in the extensive literature on determinants of differential operators.

2 Examples

Consider the *Schrödinger equation* describing a non-relativistic particle of mass m and charge e moving in three dimensional space and interacting with an external vector- and scalar potential $\mathbf{A}$ and ϕ,

$$\mathrm{i}\partial_t\psi = H\psi, \quad H = \frac{1}{2m}(-\mathrm{i}\nabla + e\mathbf{A})^2 - e\phi \tag{1}$$

(we set $\hbar = c = 1$, $\partial_t = \partial/\partial t$, and ψ, ϕ and $\mathbf{A}$ can depend on the space and time variables $\mathbf{x} \in \mathbb{R}^3$ and $t \in \mathbb{R}$). This is a standard quantum mechanical model, with ψ the one-particle wave function allowing for the usual probabilistic interpretation. One interesting generalization to the relativistic regime is the *Klein-Gordon equation*

$$\left[(\mathrm{i}\partial_t + e\phi)^2 - (-\mathrm{i}\nabla + e\mathbf{A})^2 - m^2\right]\psi = 0 \tag{2}$$

with a $\mathbb{C}$-valued function ψ. There is another important relativistic generalization, the *Dirac equation*

$$\left[(\mathrm{i}\partial_t + e\phi) - (-\mathrm{i}\nabla + e\mathbf{A})\cdot\boldsymbol{\alpha} + m\beta\right]\psi = 0 \tag{3}$$

with $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β hermitian 4×4 matrices satisfying the relations

$$\alpha_i\alpha_j + \alpha_j\alpha_i = \delta_{ij}, \quad \alpha_i\beta = -\beta\alpha_i, \quad \beta^2 = 1 \tag{4}$$

and a $\mathbb{C}^4$-valued function ψ (we write 1 also for the identity). These two relativistic equations differ by the transformation properties of ψ under Lorentz transformations: in (2) it transforms like a scalar and thus describes spin-0 particles, and it transforms like a spinor describing spin-$\frac{1}{2}$ particles in (3). While these equations are natural relativistic generalizations of the Schrödinger equation, they no longer allow to consistently interpret ψ as one-particle wave functions. The physical reason is that, in a relativistic theory, high energy processes can create particle-antiparticle pairs, and this makes the restriction to a fixed particle number inconsistent. This problem can be remedied by constructing a many-body model allowing for an arbitrary number of particles and anti-particles. The requirement that this many-body model should have a groundstate is an important ingredient in this construction.

It is obviously of interest to formulate and study many-body models of non-distinguishable already in the non-relativistic case. An important empirical fact is that such particles come in two kinds, *bosons* and *fermions*, distinguished by their exchange statistics (we ignore the interesting possibility of exotic statistics). For example, the fermion many-particle version of (1) for suitable ϕ and $\mathbf{A}$ is a useful model for electrons in a metal. An elegant method to go from the one- to the many-particle description is the formalism of *second quantization*: one promotes ψ to a quantum field operator with certain (anti-) commutator relations, and this is a convenient way to construct the appropriate many-particle Hilbert space, Hamiltonian, etc. In the non-relativistic case, this formalism can be regarded as an elegant reformulation of a pedestrian construction of a many-body quantum mechanical model, which is useful since it provides convenient computational tools. However, this formalism naturally generalizes to the relativistic case where the one-particle model no longer has an acceptable physical interpretation, and one finds that one can nevertheless can give a consistent physical interpretation to (2) and (3) provided that ψ are interpreted as quantum field operators describing bosons and fermions, respectively. This particular exchange statistics of the relativistic particles is a special case of the *spin-statistics theorem*: integer spin particles are bosons and half-integer spin particles are fermions. While many structural features of this formalism are present already in the simpler non-relativistic models, the relativistic models add some non-trivial features typical for quantum field theories.

In the following we discuss a precise mathematical formulation of the quan-

tum field theory models described above. We emphasis the functorial nature of this construction which makes manifest that it also applies to other situations, e.g., where the bosons and fermions are also coupled to a gravitational background, are considered in other spacetime dimensions than $3+1$, etc.

3 Second quantization: non-relativistic case

Consider a quantum system of non-distinguishable particles where the quantum mechanical description of one such particle is known. In general, this one-particle description is given by a Hilbert space h and one-particle observables and transformations which are self-adjoint and unitary operators on h, respectively. The most important observable is the Hamiltonian H. We will describe a general construction of the corresponding many-body system.

Example. As a motivating example we take the Hilbert space $h = L^2(\mathbb{R}^3)$ of square-integrable functions $f(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$, and the Hamiltonian H in (1). A specific example for a unitary operator on h is the gauge transformation $(Uf)(\mathbf{x}) = \exp(\mathrm{i}\chi(\mathbf{x}))f(\mathbf{x})$ with χ a smooth, real-valued functions on $\mathbb{R}^3$.

In this example, the corresponding wave functions for N identical such particles are the L^2-functions $f_N(\mathbf{x}_1, \ldots, \mathbf{x}_N)$, $\mathbf{x}_j \in \mathbb{R}^3$. It is obvious how to extend one-particle observables and transformations to such N-particle states: for example, the N-particle Hamiltonian corresponding to H in (1) is

$$H_N = \sum_{j=1}^{N} \frac{1}{2m}(-\mathrm{i}\nabla_{\mathbf{x}_j} + e\mathbf{A}(t, \mathbf{x}_j))^2 - e\phi(t, \mathbf{x}_j), \tag{5}$$

and the N-particle gauge transformation U_N is defined through multiplication with $\prod_{j=1}^{N} \exp(\mathrm{i}\chi(\mathbf{x}_j))$.

For systems of indistinguishable particles it is enough to restrict to wave functions which are even or odd under particle exchanges,

$$f_N(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_N) = \pm f_N(\mathbf{x}_1, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N) \tag{6}$$

for all $1 \leq j < k \leq N$, with the upper and lower sign corresponding to bosons and fermions, respectively (this empirical fact is usually taken as postulate in non-relativistic many-body quantum physics). It is convenient to define the zero-particle Hilbert space as $\mathbb{C}$ (complex numbers) and to introduce

a Hilbert space containing states with all possible particle numbers: This so-called *Fock space* contains all states

$$\begin{pmatrix} f_0 \\ f_1(\mathbf{x}_1) \\ f_2(\mathbf{x}_1, \mathbf{x}_2) \\ f_3(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \\ \vdots \end{pmatrix} \tag{7}$$

with $f_0 \in \mathbb{C}$. The definition of H_N and U_N then naturally extends to this Fock space; see below.

General construction. The construction of Fock spaces and many-particle observables and transformations just outlined in a specific example is conceptually simple. An alternative, more efficient construction method is to use *quantum fields* which we denote as $\psi(\mathbf{x})$ and $\psi^\dagger(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$. They can be fully characterized by the following (anti-) commutator relations,

$$[\psi(\mathbf{x}), \psi^\dagger(\mathbf{y})]_\mp = \delta^3(\mathbf{x} - \mathbf{y}), \quad [\psi(\mathbf{x}), \psi(\mathbf{y})]_\mp = 0, \tag{8}$$

where $[a, b]_\mp \equiv ab \mp ba$, with the commutator and anti-commutators (upper and lower signs) corresponding to the boson and fermion case, respectively. It is convenient to 'smear' these fields with one-particle wave functions and define

$$\psi(f) = \int_{\mathbb{R}^3} \mathrm{d}^3x \, \overline{f(\mathbf{x})} \psi(\mathbf{x}), \quad \psi^\dagger(f) = \int_{\mathbb{R}^3} \mathrm{d}^3x \, \psi^\dagger(\mathbf{x}) f(\mathbf{x}) \tag{9}$$

for all $f \in h$. Then the relations characterizing the field operators can be written as

$$[\psi(f), \psi^\dagger(g)]_\mp = (f, g), \quad [\psi(f), \psi(g)]_\mp = 0 \quad \forall f, g \in h \tag{10}$$

where $(f, g) = \int_{\mathbb{R}^3} \mathrm{d}^3x \, \overline{f(\mathbf{x})} g(\mathbf{x})$ is the inner product in h. The Fock space $\mathcal{F}_\mp(h)$ can then be defined by postulating that it contains a normalized vector Ω called *vacuum* such that

$$\psi(f)\Omega = 0 \quad \forall f \in h \tag{11}$$

and that all $\psi^{(\dagger)}(f)$ are operators on $\mathcal{F}_\mp(h)$ such that $\psi^\dagger(f) = \psi(f)^*$ where $*$ is the Hilbert space adjoint. Indeed, from this we conclude that $\mathcal{F}_\mp(h)$, as vector space, is generated by

$$f_1 \wedge f_2 \wedge \cdots \wedge f_N \equiv \psi^\dagger(f_1)\psi^\dagger(f_2) \cdots \psi^\dagger(f_N)\Omega \tag{12}$$

with $f_j \in h$ and $N = 0, 1, 2, \ldots$, and that the Hilbert space inner product of such vectors is

$$\langle f_1 \wedge f_2 \wedge \cdots \wedge f_N, g_1 \wedge g_2 \wedge \cdots \wedge g_M \rangle = \delta_{N,M} \sum_{P \in S_N} (\pm 1)^{|P|} \prod_{j=1}^{N} (f_j, g_{Pj}) \quad (13)$$

with S_N the permutation group, with $(+1)^{|P|} = 1$ always and $(-1)^{|P|} = +1$ and -1 for even and odd permutations, respectively. The many-body Hamiltonian $q(H)$ corresponding to the one-particle Hamiltonian H now can be defined by the following relations,

$$q(H)\Omega = 0, \quad [q(H), \psi^\dagger(f)] = \psi^\dagger(Hf) \quad (14)$$

for all $f \in h$ such that Hf is defined. Indeed, this implies

$$q(H) f_1 \wedge f_2 \wedge \cdots \wedge f_N = \sum_{j=1}^{N} f_1 \wedge f_2 \wedge \cdots \wedge (Hf_j) \wedge \cdots \wedge f_N \quad (15)$$

which defines a self-adjoint operator on $\mathcal{F}_\mp(h)$, and it is easy to check that this coincides with our down-to-earth definition of H_N above. Similarly the many-body transformation $Q(U)$ corresponding to a one-particle transformation U can be defined as

$$Q(U)\Omega = \Omega, \quad Q(U)\psi^\dagger(f) = \psi^\dagger(Uf)Q(U) \quad (16)$$

for all $f \in h$, which implies

$$Q(U) f_1 \wedge f_2 \wedge \cdots \wedge f_N = (Uf_1) \wedge (Uf_2) \wedge \cdots \wedge (Uf_N) \quad (17)$$

and thus coincides with our previous definition of U_N.

While we presented the construction above for a particular example, it is important to note that it actually does not make reference to what the one-particle formalism actually is. For example, if we had a model of particles on a space $\mathcal{M}$ given by some 'nice' manifold of any dimension and with M internal degrees of freedom, we would take $h = L^2(\mathcal{M}) \otimes \mathbb{C}^M$ and replace (9) by

$$\psi(f) = \int_{\mathcal{M}} \mathrm{d}\mu(\mathbf{x}) \sum_{j=1}^{M} \overline{f_j(\mathbf{x})} \psi_j(\mathbf{x}) \quad (18)$$

and its hermitian conjugate, with the measure μ on $\mathcal{M}$ defining the inner product in h, $(f,g) = \int \mathrm{d}\mu(\mathbf{x}) \sum_j \overline{f_j(\mathbf{x})} g_j(\mathbf{x})$. With that, all formulas after (9) hold true as they stand. *Given any one-particle Hilbert space h with inner product $(\cdot,\cdot)$, observable H, and transformation U, the formulas above define the corresponding Fock spaces $\mathcal{F}_\mp(h)$ and many-body observable $q(H)$ and transformation $Q(U)$.* It is also interesting to note that this construction has various beautiful general (functorial) properties: the set of one-particle observables has a natural Lie algebra structure with the Lie bracket given by the commutator (strictly speaking: i times the commutator, but we drop the common factor i for simplicity). The definitions above imply

$$[q(A), q(B)] = q([A,B]) \tag{19}$$

for one-particle observables A, B, i.e., the above-mentioned Lie algebra structure is preserved under this map q. In a similar manner, the set of one-particle transformations has a natural group structure preserved by the map Q,

$$Q(U)Q(V) = Q(UV), \quad Q(U)^{-1} = Q(U^{-1}). \tag{20}$$

Moreover, if A is self-adjoint, then $\exp(\mathrm{i}A)$ is unitary, and one can show that

$$Q(\exp(\mathrm{i}A)) = \exp(\mathrm{i}q(A)). \tag{21}$$

For later use we note that, if $\{f_n\}_{n\in\mathbb{Z}}$ is some complete, orthonormal basis in h, then operators A on h can be represented by infinite matrices $(A_{mn})_{m,n\in\mathbb{Z}}$ with $A_{mn} = (f_m, Af_n)$, and

$$q(A) = \sum_{m,n} A_{mn} \psi_m^\dagger \psi_n \tag{22}$$

where $\psi_n^{(\dagger)} = \psi^{(\dagger)}(f_n)$ obey

$$[\psi_m, \psi_n^\dagger]_\mp = \delta_{m,n}, \quad [\psi_m, \psi_n^\dagger]_\mp = 0 \tag{23}$$

for all m, n. We also note that, in our definition of $q(A)$, we made a convenient choice of normalization, but there is no physical reason to not choose a different normalization and define

$$q'(A) = q(A) - b(A) \tag{24}$$

where b is some linear function mapping self-adjoint operators A to real numbers. For example, one may wish to use another reference vector $\tilde{\Omega}$ instead of Ω in the Fock space, and then would choose $b(A) = \langle \tilde{\Omega}, q(A)\tilde{\Omega}\rangle$. Then the relation in (19) are changed to

$$[q'(A), q'(B)] = q'([A, B]) + S_0(A, B) \tag{25}$$

where $S_0(A, B) = b([A, B])$. However, the $\mathbb{C}$-number term $S_0(A, B)$ in the relations (25) is trivial since it can be removed by going back to $q(A)$.

Physical interpretation. The Fock space $\mathcal{F}_\mp(h)$ is the direct sum of subspaces of states with different particle numbers N,

$$\mathcal{F}_\mp(h) = \bigoplus_{N=0}^{\infty} h_\mp^{(N)} \tag{26}$$

where the zero-particle subspace $h_\mp^{(0)} = \mathbb{C}$ is generated by the vacuum Ω, and $h_\mp^{(N)}$ is the N-particle subspace generated by the states $f_1 \wedge f_2 \wedge \ldots \wedge f_N$, $f_j \in h$. We note that

$$\mathcal{N} \equiv q(1) \tag{27}$$

is the *particle number operator*, $\mathcal{N}F_N = NF_N$ for all $f_N \in h_\mp^{(N)}$. The field operators obviously change the particle number: $\psi^\dagger(f)$ increases the particle number by one (maps $h_\mp^{(N)}$ to $h_\mp^{(N+1)}$), and $\psi(f)$ decreases it by one. Since every $f \in h$ can be interpreted as one-particle state, it is natural to interpret $\psi^\dagger(f)$ and $\psi(f)$ as *creation* and *annihilation operators*, respectively: they create and annihilate one particle in the state $f \in h$. It is important to note that, in the fermion case, (10) implies $\psi^\dagger(f)^2 = 0$, which is a mathematical formulation of the *Pauli exclusion principle*: it is not possible to have two fermions in the same one-particle state. In the boson case there is no such restriction. Thus, even though the formalisms used to describe boson- and fermion systems look very similar, they describe dramatically different physics.

Applications. In our example, the many-body Hamiltonian $\mathcal{H}_0 \equiv q(H)$ can also be written in the following suggestive form,

$$\mathcal{H}_0 = \int \mathrm{d}^3x \, \psi^\dagger(\mathbf{x})(H\psi)(\mathbf{x}), \tag{28}$$

and similar formulas hold true for other observables and other Hilbert spaces $h = L^2(\mathcal{M}) \otimes \mathbb{C}^n$. It is rather easy to solve the model defined by such Hamiltonian: all necessary computations can be reduced to one-particle computations. For example, in the static case where $\mathbf{A}$ and ϕ are time independent, a main quantity of interest in statistical physics is the free energy

$$\mathcal{E} \equiv -\beta^{-1} \log \left(\mathrm{Tr} \left(\exp \left(-\beta [\mathcal{H}_0 - \mu \mathcal{N}] \right) \right) \right) \tag{29}$$

where $\beta > 0$ here is the inverse temperature, μ the chemical potential, and the trace over the Fock space $\mathcal{F}_{\mp}(h)$. One can show that

$$\mathcal{E} = \pm \mathrm{tr} \left(\beta^{-1} \log(1 \mp \exp(-\beta[H - \mu])) \right) \tag{30}$$

where the trace here is over the one-particle Hilbert space h. Thus, to compute $\mathcal{E}$, one only needs to find the eigenvalues of H.

It is important to mention that the framework discussed here is not only for external field problems but can be equally well used to formulate and study more complicated models with interparticle interactions. For example, while the model with the Hamiltonian $\mathcal{H}_0$ above is often too simple to describe systems in nature, it is easy to write down more realistic models, e.g., the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + (e^2/2) \int \mathrm{d}^3 x \int \mathrm{d}^3 y \, \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{y}) |\mathbf{x} - \mathbf{y}|^{-1} \psi(\mathbf{y}) \psi(\mathbf{x}) \tag{31}$$

describes electrons in an external electromagnetic field interacting through Coulomb interactions. This illustrates an important point which we would like to stress: the task in quantum theory is two-fold, namely to *formulate* and to *solve* (exact of otherwise) models. Obviously, in the non-relativistic case, it is equally simple to formulate many-body models with and without inter-particle interactions, and the latter only are simpler because they are easier to solve: the two tasks of formulating and solving models can be clearly separated. As we will see, in the relativistic case, even the formulation of an external field problem is non-trivial, and one finds that one cannot formulate the model without at least partially solving it. This is a common feature of quantum field theories making them challenging and interesting.

4 Relativistic fermion and boson systems

We now generalize the formalism developed in the previous section to the relativistic case.

Field algebras and quasi-free representations. In the previous section we identified the field operators $\psi^{(\dagger)}(f)$ with particular Fock space operators. This is analog to identifying the operators $p_j = -\mathrm{i}\partial_{x_j}$ and $q_j = x_j$ on $L^2(\mathbb{R}^M)$ with the generators of the Heisenberg algebra, as usually done. (We recall: the Heisenberg algebra is the star algebra generated by P_j and Q_j, $j = 1, 2, \ldots, M < \infty$, with the well-known relations,

$$[P_j, P_k] = -\mathrm{i}\delta_{jk}, \quad [P_j, P_k] = [P_j, Q_k] = 0, \quad P_j^\dagger = P_j\,, \quad Q_j^\dagger = Q_j \tag{32}$$

for all j, k.) Identifying the Heisenberg algebra with a particular representation is legitimate since, as is well-known, all its irreducible representations are (essentially) the same (this statement is made precise by a celebrated theorem due to von Neumann).

However, in case of the algebra generated by the field operators $\psi^{(\dagger)}(f)$, there exist representations which are truly different from the ones discussed in the last section, and to construct relativistic external field problems such representations are needed. It is therefore important to distinguish the fields as generators of an algebra from the operators representing them. We thus define the *(boson or fermion) field algebra* $\mathcal{A}_\mp(h)$ over a Hilbert space h as the star algebra generated by $\Psi^\dagger(f)$, $f \in h$, such that the map $f \to \Psi(f)$ is linear and the relations

$$[\Psi(f), \Psi^\dagger(g)]_\mp = (f, g), \quad [\Psi(f), \Psi(g)]_\mp = 0, \quad \Psi^\dagger(f)^\dagger = \Psi(f) \tag{33}$$

are fulfilled for all $f, g \in g$, with $\dagger$ the star operation in $\mathcal{A}_\mp(h)$.

The particular representation of this algebra discussed in the last section will be denoted by π_0, $\pi_0(\Psi^{(\dagger)}(f) = \psi^{(\dagger)}(f)$. Other representations π_{P_-} can be constructed from any projection operators P_- on h, i.e., any operator P_- on h satisfying $P_-^* = P_-^2 = P_-$. Writing $\hat\psi^{(\dagger)}(f)$ short for $\pi_{P_-}(\Psi^{(\dagger)}(f))$, this so-called *quasi-free representation* is defined by

$$\hat\psi^\dagger(f) = \psi^\dagger(P_+ f) + \psi(\overline{P_- f}), \quad \hat\psi(f) = \psi(P_+ f) \mp \psi^\dagger(\overline{P_- f}) \tag{34}$$

where the bar means complex conjugation. It is important to note that, while the star operation is identical with the Hilbert space adjoint $*$ in the fermion case, we have

$$\hat{\psi}(f)^\dagger = \psi(Ff)^* \text{ with } F = P_+ - P_- \text{ for bosons} \tag{35}$$

where F is a grading operator, i.e., $F^* = F$ and $F^2 = 1$. We stress that the 'physical' star operation always is $*$, i.e., physical observables A obey $A = A^*$.

The present framework suggests to regard quantization as the procedure which amounts to going from a one-particle Hilbert space h to the corresponding field algebra $\mathcal{A}_\mp(h)$. Indeed, the Heisenberg algebra is identical with the boson field algebra $\mathcal{A}_-(\mathbb{C}^M)$ (since the latter is obviously identical with the algebra of M harmonic oscillators), and thus conventional quantum mechanics can be regarded as boson quantization in the special case where the one-particle Hilbert space is finite dimensional. It is interesting to note that 'fermion quantum mechanics' $\mathcal{A}_-(\mathbb{C}^M)$ is the natural framework for formulating and studying lattice fermion and spin systems which play an important role in condensed matter physics.

In the following we elaborate the naive interpretations of the relativistic equations in (2) and (3) as a quantum theory of one particle, and we discuss why they are unphysical. For simplicity we assume that the electromagnetic fields $\phi, \mathbf{A}$ are time independent. We then show that quasi-free representations as discussed above can provide physically acceptable many-particle theories. We first consider the Dirac case which is somewhat simpler.

4.1 Fermions

One-particle formalism: Recalling that $\mathrm{i}\partial_t$ is the energy operator, we define the Dirac Hamiltonian D by rewriting (3) in the following form,

$$\mathrm{i}\partial_t\psi = D\psi, \quad D = (-\mathrm{i}\nabla + e\mathbf{A})\cdot\boldsymbol{\alpha} + m\beta - e\phi. \tag{36}$$

This Dirac Hamiltonian is obviously is a self-adjoint operator on the one-particle Hilbert space $h = L^2(\mathbb{R}^4)\otimes\mathbb{C}^4$, but, different from the Schrödinger Hamiltonian in (1), it is not bounded from below: for any $E_0 > -\infty$ one can find a state f such that the energy expectation value (f, Df) is less than E_0.

This can be easily seen for the simplest case where the external potential vanishes, $\mathbf{A} = \phi = 0$. Then the eigenvalues of D can be computed by Fourier transformation, and one finds

$$E = \pm\sqrt{\mathbf{p}^2 + m^2}, \quad \mathbf{p} \in \mathbb{R}^3. \tag{37}$$

Due to the negative energy eigenvalues we conclude that there is no ground state, and the Dirac Hamiltonian thus describes an unstable system which is physically meaningless.

To summarize: a (unphysical) one-particle description of relativistic fermions is given by a Hilbert space h together with a self-adjoint Hamiltonian D unbounded from below. Other observables and transformations are given by self-adjoint and unitary operators on h, respectively.

Many-body formalism: We now explain how to construct a physical many-body description from these data. To simplify notation we first assume that D has a purely discrete spectrum (which can be achieved by using a compact space). We then can label the eigenfunctions f_n by integers n such that the corresponding eigenvalues $E_n \geq 0$ for $n \geq 0$ and $E_n < 0$ for $n < 0$. Using the naive representation of the fermion field algebra discussed in the last section we get (we use the notation introduced in (22))

$$q(D) = \sum_{n\geq 0} |E_n| \psi_n^\dagger \psi_n - \sum_{n<0} |E_n| \psi_n^\dagger \psi_n, \tag{38}$$

which is obviously not bounded from below and thus not physically meaningful. However, $\psi_n^\dagger \psi_n = 1 - \psi_n \psi_n^\dagger$, which suggests that we can remedy this problem by interchanging the creation- and annihilation operators for $n < 0$. This is possible: it is easy to see that

$$\hat{\psi}_n \equiv \psi_n \quad \forall n \geq 0 \;\text{ and }\; \hat{\psi}_n \equiv \psi_n^\dagger \quad \forall n < 0 \tag{39}$$

provides a representation of the algebra in (23). We thus define

$$\hat{q}(D) \equiv \sum_{n\in\mathbb{Z}} E_n : \hat{\psi}_n^\dagger \hat{\psi}_n : \tag{40}$$

with the so-called *normal ordering* prescription

$$: \psi_m^\dagger \psi_n : \equiv \psi_m^\dagger \psi_n - \langle \Omega, \psi_m^\dagger \psi_n \Omega \rangle, \tag{41}$$

where we made use of the freedom of normalization explained after (23) to eliminate unwanted additive constants. We get $q(D) = \sum_{n\in\mathbb{Z}} |E_n|\psi_n^\dagger\psi_n$, which is manifestly a non-negative self-adjoint operator with Ω as ground-state. We thus found a physical many-body description for our model. We now can define for other one-particle observables,

$$\hat{q}(A) \equiv \sum_{n\in\mathbb{Z}} A_{mn} :\hat{\psi}_m^\dagger\hat{\psi}_n:, \tag{42}$$

and by straightforward computations we obtain

$$[\hat{q}(A), \hat{q}(B)] = \hat{q}([A,B]) + S(A,B) \tag{43}$$

where $S(A,B) = \sum_{m<0}\sum_{n\geq 0}(A_{mn}B_{nm} - B_{mn}A_{nm})$, i.e.,

$$S(A,B) = \mathrm{tr}\,(P_-AP_+BP_- - P_-BP_+AP_-) \tag{44}$$

with $P_- = \sum_{n<0} f_n(f_n,\cdot)$ the projection onto the subspace spanned by the negative energy eigenvectors of D and $P_+ = 1 - P_-$. One can show that $\hat{q}(A)$ no longer is defined for *all* operators but only if

$$P_-AP_+ \;\text{ and }\; P_+AP_- \;\text{ are Hilbert-Schmidt operators} \tag{45}$$

(we recall that a is a Hilbert-Schmidt operator if $\mathrm{tr}(a^*a) < \infty$). The $\mathbb{C}$-number term $S(A,B)$ in (43) is often called *Schwinger term*, and different from the similar term in (25) it now is non-trivial, i.e., it no longer is possible to remove it be a redefinition $\hat{q}'(A) = \hat{q}(A) - b(A)$. This Schwinger term is an example of an anomaly, and it has various interesting implications.

In a similar manner, one can construct the many-body transformations $\hat{Q}(U)$ of unitary operators U on h satisfying the very Hilbert-Schmidt condition in (45), and one obtains

$$\hat{Q}(U)\hat{Q}(V) = \chi(U,V)\hat{Q}(UV) \tag{46}$$

with an interesting phase valued functions χ.

More generally, for any one-particle Hilbert space h and Dirac Hamiltonian D, the physical representation is given by the quasi-free representation π_{P_-} in (34) with P_- the projection onto the negative energy subspace of D. The results about $\hat{q}$ and $\hat{Q}$ mentioned hold true in any such representation.

Thus the one-particle Hamiltonian D determines which representation one has to use, and one therefore cannot construct the 'physical' representation without specific information about D. However, not all these representations are truly different: If there is a unitary operator $\mathcal{U}$ on the Fock space $\mathcal{F}_+(h)$ such that

$$\mathcal{U}^* \pi_{P_-^{(1)}}(\psi^{(\dagger)}(f))\mathcal{U} = \pi_{P_-^{(2)}}(\psi^{(\dagger)}(f)) \tag{47}$$

for all $f \in h$, then the quasi-free representations associated with the different projections $P_-^{(1)}$ and $P_-^{(2)}$ are physically equivalent: one could equally well formulate the second model using the representation of the first. Two such quasi-free representations are called *unitarily equivalent*, and a fundamental *theorem* due to *Shale and Stinespring* states that two quasi-free representations $\pi_{P_-^{(1,2)}}$ are unitarily equivalent if and only if $P_-^{(1)} - P_-^{(2)}$ is a Hilbert-Schmidt operator (a similar result holds true in the boson case).

4.2 Bosons

One-particle formalism: Similarly as for the Dirac case, also the solutions of the Klein-Gordon equation in (2) do not define a physically acceptable one-particle quantum theory with a ground state: the energy eigenvalues in (37) for $\mathbf{A} = \phi = 0$ are a consequence the relativistic invariance and thus equally true for the Klein-Gordon case. However, in this case there is a further problem. To find the one-particle Hamiltonian one can rewrite the second order equation in (2) as a system of first order equations,

$$\mathrm{i}\partial_t \Phi = K\Phi, \quad \Phi = \begin{pmatrix} \psi \\ \pi^\dagger \end{pmatrix}, \quad K = \begin{pmatrix} C & \mathrm{i} \\ -\mathrm{i}B^2 & C \end{pmatrix} \tag{48}$$

with

$$B^2 \equiv (-\mathrm{i}\nabla + e\mathbf{A})^2 + m^2, \quad C \equiv -e\phi. \tag{49}$$

Thus one sees that the natural one-particle Hilbert space for the Klein-Gordon equation is $h = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$; here and in the following we identify h with $h_0 \oplus h_0$, $h_0 = L^2(\mathbb{R}^3)$, and use a convenient 2×2 matrix notation naturally associated with that splitting. However, the one-particle Hamiltonian is not self-adjoint but rather obeys

$$K^* = JKJ, \quad J \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \tag{50}$$

with $*$ the Hilbert space adjoint. It is important to note that J is a grading operator. Thus, we can define a sequilinear form

$$(f, g)_J \equiv (f, Jg) \quad \forall f, g \in h, \tag{51}$$

with $(\cdot, \cdot)$ the standard inner product, and (50) is equivalent to K being self-adjoint with respect to this sesquilinear form; in this case we say that K is *J-self-adjoint*. Thus, in the Klein-Gordon case, this sesquilinear form takes the role of the Hilbert space inner product and, in particular, not (Φ, Φ) but $(\Phi, \Phi)_J$ is preserved under time evolution. However, different from $\Phi^\dagger\Phi$, $\Phi^\dagger J\Phi$ is not positive definite, and it is therefore not possible to interpret it as probability density as in conventional quantum mechanics. For consistency one has to require that one-particle transformations U are unitary with respect to $(\Phi, \Phi)_J$, i.e., $U^{-1} = JUJ$. We call such operators *J-unitary*.

To summarize: a (unphysical) one-particle description of relativistic bosons is given by a Hilbert space of the form $h = h_0 \oplus h_0$, the grading operator J in (50), and a J-self-adjoint Hamiltonian K of the form as in Eq. (48) where $B \geq 0$ and C are self-adjoint operators on h_0. Other observables and transformations are given by J-self-adjoint and J-unitary operators on h, respectively.

Many-body formalism: We first consider the quasi-free representation $\pi_{P_-^{(0)}}$ of the boson field algebra $\mathcal{A}_-(h)$ so that the grading operator in (35) is equal to J, i.e., $P_-^{(0)} = (1 - J)/2$. Writing $\pi_{P_-^{(0)}}(\Psi^{(\dagger)}(f)) = \psi^{(\dagger)}(f)$ one finds that

$$q(A)^* = q(JAJ), \quad Q(U)^* = Q(JU^*J), \tag{52}$$

and thus J-selfadjoint operators and J-unitary operators are mapped to proper observables and transformations. In particular, $q(K)$ is a self-adjoint operator, which resolves one problem of the one-particle theory. However, $q(K)$ is not bounded from below, and thus $\pi_{P_-^{(0)}}$ is not yet the physical representation.

The physical representation can be constructed using the operators

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} B^{1/2} & \mathrm{i}B^{-1/2} \\ B^{1/2} & \mathrm{i}B^{-1/2} \end{pmatrix}, \quad F = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{53}$$

(for simplicity we restrict ourselves to the case $C = 0$ and $B > 0$; we use of the calculus of self-adjoint operators here) with the following remarkable

properties,

$$T^{-1} = JT^{*}F, \quad TKT^{-1} = \begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix} \equiv \hat{K}. \tag{54}$$

One can check that

$$\hat{\psi}^{\dagger}(f) \equiv \psi^{\dagger}(Tf), \quad \hat{\psi}(f) \equiv \psi(T^{-1}f), \tag{55}$$

is a quasi-free representation π_{P_-} of $\mathcal{A}_-(h)$ with $P_- = (1-F)/2$. With that the construction of $\hat{q}$ and $\hat{Q}$ is very similar to the fermion case described above (the crucial simplification is that $\hat{K}$ and F now are diagonal). In particular, $\hat{q}(K)$ is a non-negative operator with the ground state Ω, and $\hat{q}(A)$ and $\hat{Q}(U)$ is self-adjoint and unitary for every one-particle observable A and transformation U, respectively. One also gets relations as in (43) and (46).

5 Further reading

The impossibility to construct relativistic quantum mechanical models played an important role in the early history of quantum field theory, as beautifully discussed in [4], Chapter 1.

The abstract formalism of quasi-free representations of fermion and boson field algebras was developed in many papers; see e.g. [5, 6, 7] for explicit results on $\hat{Q}$ and χ. A nice textbook presentation with many references can be found in [8], Chapter 13 (this chapter is rather self-contained but mainly restricted to the fermion case).

Based on the Shale-Stinespring theorem there has been considerable amount of work to investigate whether the quasi-free representations associated with different external electromagnetic fields $\psi_1, \mathbf{A}_1$ and $\psi_2, \mathbf{A}_2$ are unitarily equivalent, if and which time dependent many-body Hamiltonians exist etc.; see [8], Chapter 13 and references therein.

The infinite dimensional Lie g_2 of Hilbert space operators satisfying the condition in (45) is an interesting infinite dimensional Lie algebra with a beautiful representation theory. This subject is closely related to conformal field theory; see e.g. [9] for a textbook presentation and [10] for a detailed mathematical account within the framework described by us.

It turns out that the mathematical framework discussed in Section 4 is sufficient for constructing fully interacting quantum field theories, in particular Yang-Mills gauge theories, in 1+1 but not in higher dimensions. The reason is that, in 3+1 dimensions, the one-particle observables A of interest do not obey the Hilbert-Schmidt condition in (45) but only the weaker condition,

$$\mathrm{tr}(a^* a)^n < \infty, \quad a = P_{\mp} A P_{\pm}. \tag{56}$$

with $n = 2$, and the natural analog of g_2 in 3+1 dimensions thus seems to be the Lie algebra g_{2n} of operators satisfying this condition with $n = 2$. Various results on the representation theory of such Lie algebras $g_{2n>2}$ have been developed; see [11] where also various interesting relations to infinite dimensional geometry are discussed.

As mentioned, the Schwinger term $S(A, B)$ in (44) is an example of an anomaly. Mathematically it is a non-trivial 2-cocycles of the Lie algebra g_2, and analogs for the groups $g_{2n>2}$ have been found. These cocycles provide a natural generalization of anomalies (in the meaning of particle physics) to operator algebras. They not only shed some interesting light on the latter, but also provide a link to notions and results from non-commutative geometry; see e.g. [8]. We believe that this link can provide a fruitful driving force and inspiration to find ways to deepen our understanding of quantum Yang-Mills theories in 3+1 dimensions [12].

Keywords

Conformal field theory
anomalies
Noncommutative geometry
Dirac operators
Determinants of differential operators

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